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# Structural and electronic characterization of $(2,3_3)$ bar-shaped stacking fault in 4H-SiC epitaxial layers

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Crystallographic, electronic, and energetic analyses of the $(2,3_3)$ [or (2,3,3,3) in the standard Zhadanov notation] bar-shaped stacking fault, observed in as-grown 4H-SiC epitaxial layers, are presented. The defect has been identified by means of spatially resolved microphotoluminescence ($\mu$-PL) measurements at different emission wavelengths, focusing on the emission peak at 0.3 eV below the conduction band. Low temperature $\mu$-PL measurements have also been performed. The defect has been identified and characterized using high resolution transmission electron microscopy. Experimental results are correlated and validated by the calculations of the Kohn–Sham electronic band structure and the defect formation energy. © *2011 American Institute of Physics*.
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Silicon carbide is considered a very promising material for the development of electronic devices with improved performance in the field of high-power and high-frequency electronics and also for high-temperature applications.[1] In the case of the 4H polytype, one of the fundamental limiting steps for the commercialization of efficient bipolar devices is the degradation of I-V characteristics due to the enlargement of single Shockley (1,3) stacking faults (SFs) in the epitaxial layers.[2] However, the single Shockley SF is not the unique (meta)stable defective structure in the 4H-SiC polytype. Indeed, in order to obtain a complete comprehension of the SF formation and evolution mechanisms, a wide ensemble of the Shockley and Frank SF types[3] has been experimentally observed[4–8] and theoretically studied.[9–12] We note that both the Shockley and Frank SFs can be generally referred as stable lamellae of different polytypes with finite thickness and lateral dimension. The joined experimental and theoretical study is a fundamental step to improve chemical vapor deposition growth processes of 4H-SiC epitaxial layers for the development of a reliable bipolar device technology. In this work a fully comprehensive analysis of a SF class characterized by low formation energy and, consequently, thermodynamic stability is reported.

The sample used for the analysis has been grown on an 8° off axis SiC substrate cut toward the $[11\bar{2}0]$ direction by using silane and propane as precursor gases.[13] The growth rate was 20 $\mu$m/h and the average sample thickness was approximately 55 $\mu$m. $\mu$-PL mapping is a nondestructive technique which was applied to identify the type and morphology of stacking faults on as-grown samples. The presence of a SF has the effect to lower, locally, the intensity of the photoluminescence (PL) peak associated to the band edge emission of 4H-SiC. This allows the identification of the regions of the surface where the SFs are present. Moreover, since each SF has a specific PL signature, this permits to discern the different types of SFs in the epitaxial film. $\mu$-PL mapping measurements have been performed using a *PLMicro*-SiC by *Nanometrics, Inc.* The apparatus allows spectral analysis on samples and spatially resolved $\mu$-PL intensity map at a fixed wavelength. The motorized stage has a resolution of up to 0.5 $\mu$m. The pumping source is an UV 325 nm He-Cd laser with an exit power of 50 mW. The signal is dispersed with a grating monochromator and detected by a photomultiplier. High resolution transmission electron microscopy (HR-TEM) analyses have been obtained by using a JEOL JEM 2010F with a field emission gun. The results of $\mu$-PL characterization are shown in Fig. 1. Figure 1(a) shows an intensity map collected at room temperature at 2.9 eV (i.e., about 0.3 eV from the bottom of the conduction band). Figure 1(b) shows the corresponding low temperature PL signature with, in inset, the room temperature spectrum. These PL signatures correspond clearly to the same 2.95 eV defect signatures reported in Refs. 7 and 14.

In order to confirm the crystallographic structure of this defect, a HR-TEM analysis was done. The sample has been prepared to perform a cross-section analysis and oriented in order to intercept defects coming toward the surface. The HR-TEM image (see Fig. 2) allowed the individuation of the defect stacking sequence which, using the standard Zhadanov notation, can be referred as a (2,3,3,3) SF. It is the result of a coalescence of the two Shockley plus one Frank-type SFs. Indeed, (a) using Hagg's notation we have (++−−++−−++−−) for the 4H polytype sequence, (b) with a first Shockley fault we obtain the following sequence (++−−−+−−++−−), (c) with a second Shockley fault in the same shear direction we have (++−−−+−−+−−−), and (d), finally, applying a Frank-type fault, we get (++−−−+++−−−), i.e., the (2,3,3,3) defect using the Zadhanov notation. This fault is made of three half unit cells of 6H-SiC embedded in the

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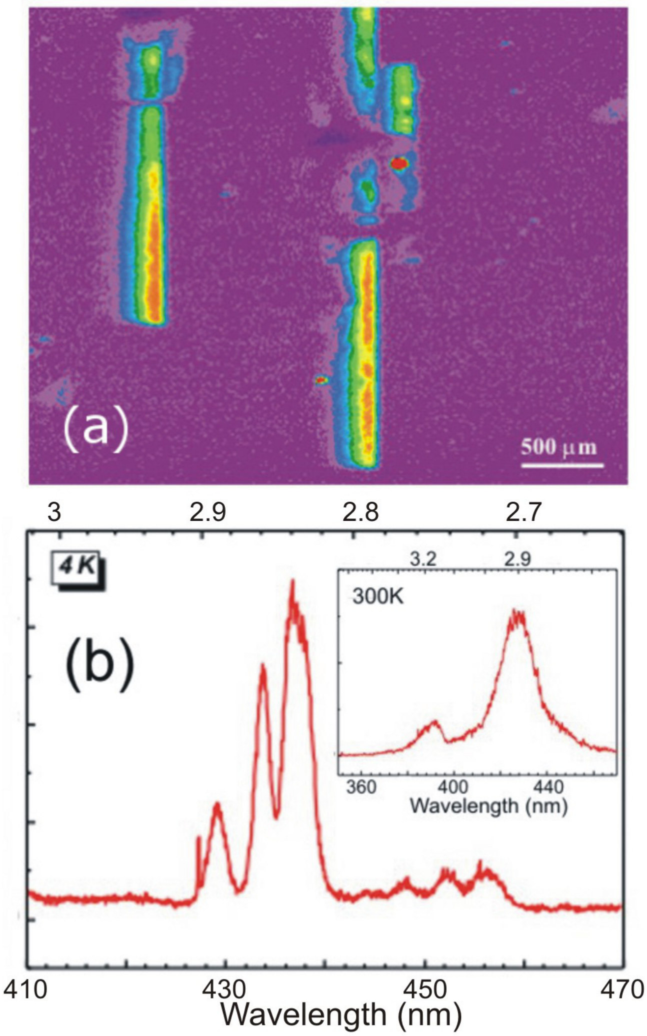


FIG. 1. (Color online) (a) Extended microphotoluminescence map at room temperature at 2.9 eV. (b) Low temperature PL and room temperature PL (inset) peaks of the defect.

4H-SiC matrix and belongs to a class of defects that can be generically considered as 3C-SiC zigzag inclusions.[14] To emphasize this aspect and to use a more compact notation, we suggest the following modified representation: $(2,3_{\mathrm{m}})$, with m indicating the number of 3C-like lamellae. This representation is similar to the one used in Ref. 14 but it clearly shows the difference between a standard single Shockley stacking fault (1,3) and the (2,3) [$(2,3_1)$ in the modified notation].

We have numerically evaluated the electronic structure and energetic of this defect using the Vienna *ab initio* simulation package (VASP) in order to demonstrate that the PL peak at 2.9 eV can be correctly attributed to $(2,3_3)$ SF. The electronic and energetic properties of the defect have been calculated by a total energy and force density functional approach using the gradient corrected functional of Perdew and Wang,[15] which was proven to be an accurate numerical framework to describe bulk[16] and surface properties[16,17] of silicon carbide. The Kohn–Sham equations are cast and solved with the projector augmented wave approach.[18,19] Both in C as in Si the outer p and s electrons are treated variationally, leaving core electrons frozen in their atomic states. A plane wave basis set of 280 eV was adopted to

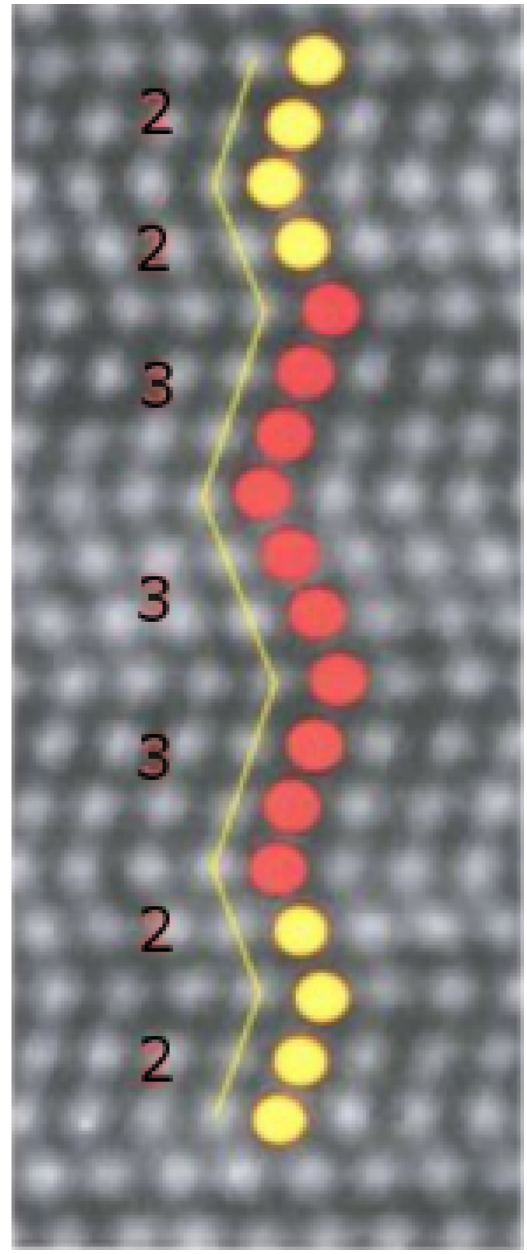


FIG. 2. (Color online) High-resolution TEM image of the $(2,3_3)$ stacking fault.

reach full convergence. The two-dimensional defects were embedded in a three-dimensional periodic superlattice containing up to 192 atoms (i.e., 24 unit cells along the [0001] direction). Moreover, to recover the correct periodicity of the supercell, a second $(2,3_3)$ stacking fault with opposite shear direction was also generated into the computational box. The distance between the two SFs has been tuned in order to make negligible their interaction. Convergence in the geometry optimization was achieved when the forces between the ions were smaller than $10^4$ eV/Å. Upon convergence, the formation energy of the defect was determined to be as low as $\sim 2$ mJ/m$^2$.

In Fig. 3 the Kohn–Sham electronic band structures of the pure 4H crystal and the $(2,3_3)$ defect are shown. An arrow indicates the energy levels inside the band gap at the M point due to the presence of the defect. Three separated levels have been generated by the defect, but only the lowest one can be detected in the PL signal due to the fast thermal-

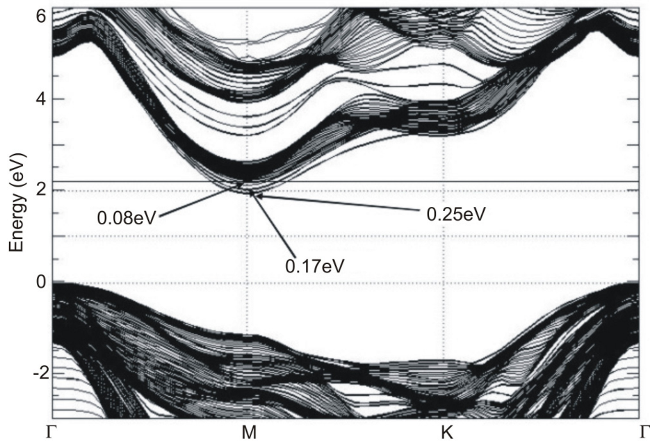


FIG. 3. Kohn–Sham band structures along the closed path Γ-M-K-Γ in the Brillouin zone of the defect supercell. The arrows indicate the intragap energy levels generated by the defect, responsible of the PL peak at 2.9 eV.

ization of electrons to the lowest level. The lowest intragap level was found to be 0.243 eV below the conduction band edge in very good agreement with the experimentally observed one at about 0.3 eV and in good agreement with the one calculated in Ref. 14 using the quantum well model, further supporting the idea that this class of defects can be considered as 6H inclusions within the 4H polytype.

In summary an unidentified PL peak at 2.9 eV has been observed on as-grown 4H-SiC epitaxial layers. An accurate optical and structural characterization of the defect allowed to associate this peak to the $(2,3_3)$ bar-shaped stacking fault which can be considered the coalescence of two Shockley plus one Frank-type stacking faults. The experimental data have been confirmed by theoretical simulations which allowed also to determine the defect formation energy which was found to be lower than any other stacking fault considered so far.[3,11,12]

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